

Pregnanolone TMS

Inchi: InChI=1S/C24H42O2Si/c1-16(25)20-9-10-21-19-8-7-17-15-18(26-27(4,5)6)11-13-23(17,24)22
InchiKey: GKHYMQSZBQGVKC-IYJLHAMFSA-N
Formula: C24H42O2Si
SMILES: CC(=O)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 390.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.29		Crippen Method
logp	6.454		Crippen Method
rinpol	2658.00		NIST Webbook
rinpol	2675.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R580166&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/49-750-5/Pregnanolone-TMS.pdf>

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